e) Rotational invariance of the Hamiltonian of the reduced one body problem

CENTRAL POTENTIAL: POTENTIAL WHICH DEPENDS ONLY ON THE DISTANCE FROM A CENTER.

Important Chapter before introduction of angular momentum.

Separation of variables:
Angular part : Eigenstates of angular momentum operator
Radial part:

The key point is the conservation of angular momentum.
What is conserved ? ***No torque***, which is true for central potentials.
(Force and direction are parallel, $\vec{F}\,||\,\vec{r}$)
Torque thinking not useful in QM.
Answer in QM: ***Angular momentum is conserved, when there is rotational symmetry***

Clearly, with angular momentum conservation, the central potential problem becomes one of finding the simultaneous eigenstates of the Hamiltonian and the angular momentum. The knowledge of the eigenstates of the latter is then used to simplify the simultaneous eigenstate problem.
Central potential problems important in classical mechanics (***Kepler's Laws***)
Same true for QM.
Major, historically most important, central force motion in QM is the Kepler motion found in hydrogen atoms
➜ few pedagogical examples of QM motion under central potential (practice problems) with only an occasional glimpse at real world applications.
Classical Kepler problem: Two body problem. Many QM central potential problems in the real world are also two-body problems.
We know how to solve only one-body Schroedinger equation exactly.
➜ We must learn how to convert the two body problem into a doable one-body problem

Hamiltonian:

$$\hat{H} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + V\left(\left|\vec{r}_1 - \vec{r}_2\right|\right) \qquad (11.1.27)$$

which is a six-dimensional Hamiltonian.

The trick of the reduction of the two body problem is to replace the two initial bodies (m_1 and m_2) by two new bodies (M, μ) where

$$M = m_1 + m_2 \quad \text{and} \quad \frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2}$$

As we have seen , the massive particle moves free of any potential. The light particle of reduced mass, μ , moves within the central potential of interest.
Mathematically, what we do is a ***coordinate transformation*** in three dimensional space taking us to the ***center-of-mass reference frame*** defined by

$$M\vec{R} = m_1\vec{r}_1 + m_2\vec{r}_2 \qquad \vec{r} = \vec{r}_1 + \vec{r}_2$$

$$\vec{P} = \vec{p}_1 + \vec{p}_2 \qquad \underbrace{\frac{\vec{p}}{m}}_{\dot{\vec{r}}} = \underbrace{\frac{\vec{p}_1}{m_1}}_{\dot{\vec{r}}_1} - \underbrace{\frac{\vec{p}_2}{m_2}}_{\dot{\vec{r}}_2}$$

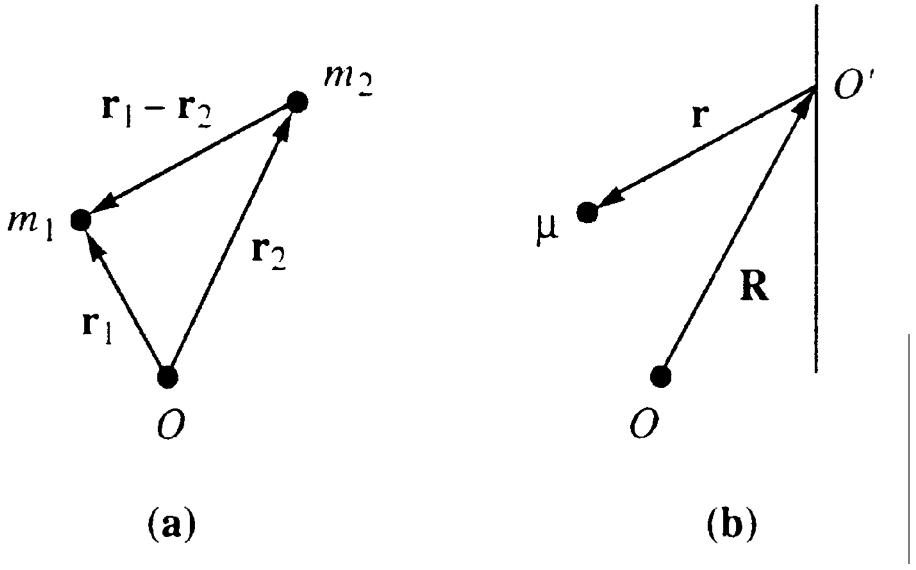

Fig. 11. 3 Transformation to the center of mass coordinate system; a) coordinate system with origin O fixed in space; b) coordinate system with origin at the center of mass (O')

In terms of these new variables,

$$\hat{H} = \frac{\hat{P}^2}{2M} + \frac{\hat{p}^2}{2m} + V\left(\left|\vec{r}\right|\right) \qquad (11.1.28)$$

This is the Hamiltonian of two independently moving particles, and therefore the reduction has been achieved. Whenever the Hamiltonian is the sum of two independent parts, the eigenvalue problem can be separated.

The Hamiltonian of the one-body Schroedinger equation for the particle μ is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V\left(\left|\vec{r}\right|\right) = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \qquad (11.1.29)$$

Let us consider the symmetry of this Hamiltonian under rotation of the coordinate system. Suppose we rotate the coordinate system about the z-axis by an angle J into a system x', y', z'

$$\begin{aligned} x' &= x\cos J - y\sin J \\ y' &= x\sin J + y\cos J \\ z' &= z \end{aligned}$$

The inverse relations are

$$\begin{aligned} x &= x'\cos J + y'\sin J \\ y &= -x'\sin J + y'\cos J \\ z &= z' \end{aligned}$$

Proof of invariance of $\hat{H}$ under this rotation

$$r' = \sqrt{x'^2 + y'^2 + z'^2} = \sqrt{x^2 + y^2 + z^2} = r$$

➜ potential does not change under rotation

$$\begin{aligned}
\nabla'^2 &= \left[(\partial / \partial x')^2 + (\partial / \partial y')^2 + (\partial / \partial z')^2\right] \\
&= \left[(\partial x / \partial x')(\partial / \partial x) + (\partial y / \partial x')(\partial / \partial y)\right]^2 \\
&\quad + \left[(\partial x / \partial y')(\partial / \partial x) + (\partial y / \partial y')(\partial / \partial y)\right]^2 \\
&\quad + (\partial / \partial z)^2 \\
&= \left[\cos J\,(\partial / \partial x) - \sin J\,(\partial / \partial y)\right]^2 \\
&\quad + \left[\sin J\,(\partial / \partial x) + \cos J\,(\partial / \partial y)\right]^2 \\
&\quad + (\partial / \partial z)^2 = \nabla^2
\end{aligned}$$

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz$$

$$\frac{df}{dx'} = \frac{\partial f}{\partial x}\frac{dx}{dx'} + \frac{\partial f}{\partial y}\frac{dy}{dx'} + \frac{\partial f}{\partial z}\frac{dz}{dx'}$$

$$\Rightarrow \frac{d}{dx'} = \left(\frac{dx}{dx'}\right)\left(\frac{\partial}{\partial x}\right) + \left(\frac{dy}{dx'}\right)\left(\frac{\partial}{\partial y}\right) + \left(\frac{dz}{dx'}\right)\left(\frac{\partial}{\partial z}\right)$$

As x is a function of x’ and y’ we can replace the total differential, d, by the partial one, ∂ .

➜ the Hamiltonian, kinetic plus potential energy, remains unchanged under rotations

If there is an invariance, there should be a conservation law, and we will see that there is an operator connected with rotation that commutes with the rotationally invariant Hamiltonian. To find the operator, consider an infinitesimal rotation about the z-axis, that is, put

$$\cos J = 1 \quad \sin J = J$$

in the transformation equations

$$\begin{aligned} x' &= x - J\,y \\ y' &= y + J\,x \qquad \text{(11.1.30)} \\ z' &= z \end{aligned}$$

Let $y\,(x, y, z)$ denote an eigenfunction of $\hat{H}$

$$\hat{H}y\,(x, y, z) = Ey\,(x, y, z) \qquad \text{(11.1.31)}$$

Now impose the condition that

$$\hat{H}y\,(x', y', z') = Ey\,(x', y', z')$$

Or, substituting for x’, y’, and z’ from (11.1.30) we have

$$\hat{H}y\,(x - J\,y, y + J\,x, z) = Ey\,(x - J\,y, y + J\,x, z)$$

Taylor expansion of ψ, and keeping terms only to first order in J and then subtract (11.1.31) yields

$$\hat{H}\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)y\,(x,y,z)=E\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)y\,(x,y,z)$$

$$=\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)\hat{H}y\,(x,y,z)$$

$$y\,(x-J\,y,y+J\,x,z)=y\,(x,y,z)$$

$$+\frac{\partial y}{\partial x}(-J\,y)+\frac{\partial y}{\partial y}(J\,x)+\frac{\partial y}{\partial z}\cdot 0$$

$$+terms\ in\,(J\,y)^2\ and\ (J\,x)^2 and\ higher\ powers$$

$$y\,(x,y,z)+J\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)y\,(x,y,z)$$

We divide by J , which is ***infinitesimal small*** but ***not zero***, and get the above result after subtracting ψ(x, y, z)

But

$$x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}=\frac{i}{\hbar}\hat{L}_z \qquad (11.1.32)$$

$\hat{L}_z$: **z-component of the angular momentum**

In this way, we see that $\hat{L}_z$ commutes with $\hat{H}$, $\left[\hat{L}_z, \hat{H}\right] = 0$, as far as operation on ψ is concerned. However, the functions ψ(x, y, z), being eigenfunctions of $\hat{H}$ form a complete and any wavefunction can be expanded in terms of them. It follows that the commutation relation

$$\left[\hat{L}_z, \hat{H}\right] = 0 \qquad (11.1.33)$$

holds true in general.

Similarly, by considering rotations about the x-axis and y-axis, we can easily show that

$$\left[\hat{H}, \hat{L}_x\right] = \left[\hat{H}, \hat{L}_y\right] = 0 \qquad (11.1.34)$$

➜ ***angular momentum conserved quantity*** we have been looking for.

Infinitesimal rotation about z-axis:

$$y\,(x', y', z') = \left(1 + \frac{i\hat{L}_z J}{\hbar}\right) y\,(x, y, z) \qquad (11.1.35)$$

$\Rightarrow \hat{L}_z$ is recognized as the ***generator of infinitesimal rotation about the z-axis***

(in the same spirit that we recognize the ***Hamiltonian***, $\hat{H}$, as the ***generator of translation in time***)

Coming back to the treatment of the central potential Hamiltonian, how do we take advantage of the conserved quantities (namely, $\hat{L}_x, \hat{L}_y, and\ \hat{L}_z$, discovered above ?)

Slight problem: these operators ***do not form a commuting set*** and therefore ***cannot ALL*** have ***simultaneous eigenvalues with*** $\hat{H}$, and ***cannot ALL*** be used as ***labels for the eigenstates of*** $\hat{H}$.

There is, however, the ***operator*** $\hat{L}^2$ ***, which commutes with all the*** $\hat{L}_i$***, (i = x, y, z) and with*** $\hat{H}$**.**

Accordingly, we seek ***simultaneous eigenvalues of*** $\hat{H}$ ***,*** $\hat{L}^2$ ***, and*** $\hat{L}_z$ (the last one by convention).

Note, that since we are going to calculate eigenstates in 3 dimensions, we must have three labels for them; the above three eigenvalues provide these labels. Now let us label the states as $|n,m,l\rangle$

n: quantum number related to energy

l: orbital quantum number; eigenvalue of $\hat{L}$ **is** $\sqrt{l(l+1)}\hbar$

m: eigenvalue of $\hat{L}_z$ **is** $m\hbar$

m = -l, -l + 1, -l + 2 ,.........., l - 1, l **l ≥ |m|**

Bound state problem ➜ no generality is lost assuming discrete energy levels

Eigenvalue equation

$$\hat{H}|n,l,m\rangle = E|n,l,m\rangle$$

in spherical coordinate representation

$$\frac{2m}{\hbar^2}\langle r,J,j\,|\hat{H}|n,l,m\rangle = \langle r,J,j\,|\frac{\hat{L}}{r^2\hbar^2} - \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{2mV(r)}{\hbar^2}|n,l,m\rangle$$

$$= \frac{2mE}{\hbar^2}\langle r,J,j\,|n,l,m\rangle \qquad (11.1.36)$$

Since the Hamiltonian contains ***additive terms*** that act on separate ***subspaces***, the ***angular and radial spaces***, respectively, the Schroedinger equation for the eigenfunction

$$\langle r,J,j\,|n,l,m\rangle = y_{nlm}(\vec{r})$$

clearly is separable in angular and radial parts, the angular part being the eigenfunction of $\hat{L}^2$. Accordingly we factorize ψ_{nlm} in the form

$$y_{nlm}(\vec{r}) = R_{nl}(r)Y_l^m(J,j) \qquad (11.1.37)$$

where the quantum number, n, (as the quantum number related to energy) will emerge from the solution of the radial equation.

$$0 = \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{2m}{\hbar^2} \{ E - V(r) \} - \frac{\hbar^2 l(l+1)}{2mr^2} \right] R_{nl}(r) \quad (11.1.38)$$

This follows from the solution of

$$\hat{L}^2 Y_l^m(J, j) = l(l+1)\hbar^2 Y_l^m(J, j) \qquad (11.1.39)$$

After this introduction we will deal with the hydrogen atom and achieve a deeper understanding before we deal with the angular momentum operator on a higher level.